Japan Geoscience Union Meeting 2012
(May 20-25 2012 at Makuhari, Chiba, Japan)

SIT42-P14 会場:コンベンションホール 時間:5 月 22 日 17:15-18:30

二次元検出器を利用した多結晶体の結晶選択配向および格子歪み解析手法の開発
Simultaneous analysis of strain and texture of polycrystalline materials using two-dimensional X-ray diffraction pattern

瀬戸 雄介 [1*]
SETO, Yusuke[1*]

[1] 神戸大学・院・理
[1]Kobe Univ. Sci.

Angle dispersive powder X-ray diffraction experiments using a two-dimensional area detector are one of the most powerful methods for Earth material sciences, particularly under high pressure conditions. A two-dimensional intensity distribution on Debye rings immediately involves information of the number of crystallites, lattice preferred orientation (LPO) and lattice strains under stress; i.e. the number of crystallites is directly related with the spottiness on the Debye rings. When a LPO is developed, diffracted intensities along the Debye rings show circumferential oscillations unique to a manner of the three-dimensional orientation distribution. The effect of lattice strain appears in elliptic distortions of the each ring or a deviation of the original crystallographic geometry between rings. These are substantial factors of the bulk physical properties of a polycrystalline material, including seismic velocity, thermal/electric conductivity and so on, but in many cases the quantitative treatments have not yet been developed into a standard technique.

In the present study, the author developed a software code, which simulates a two-dimensional diffraction pattern based on given experimental parameters (e.g. wave length, beam convergence, camera length, pixel size of a detector, and so on) and (poly)crystalline properties (crystal structure, crystallite number, size, orientation distribution, lattice strain and so on). Through the simulation, the effect of the parameters on the diffraction pattern can be quantitatively and visually estimated. Furthermore, to find the orientation distribution and the lattice strain from the observed diffraction pattern, a fitting procedure is incorporated into the code as follows: The software initially generates a large number (10^6-10^7) of crystallites with random orientation under a strain-free condition, evaluates the residual of the simulated/observed patterns, and then iteratively modifies the orientation distribution and stress condition. In each iterative step, randomly selected crystallites (0.1-1.0 %) are roughly orientated toward a randomly generated direction, and the modified distribution are (or not) adopted if the residual becomes small (or large). Components of stress tensor are also modified at several intervals. By repeating the iteration step many times ($>10^5$), the simulation seems to converge to a certain condition. A pole figure (density map of a crystallographic axis or plane direction) can be calculated from the obtained orientation distribution. The fitting procedure was applied for several actual diffraction patterns from in-situ uniaxial compression experiments, and its validity was confirmed.

キーワード: 粉末 X 線回折, 選択配向, 格子ひずみ, 二次元検出器, 多結晶体
Keywords: X-ray powder diffraction, lattice preferred orientation, lattice strain, two-dimensional detector, polycrystalline material